

Lattice thermal conductivity of ultra high temperature ceramics (UHTC) ZrB₂ and HfB₂ from atomistic simulations

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Ultra high temperature ceramics (UHTC) including ZrB₂ and HfB₂ are candidate materials for applications in extreme environments because of their high melting point, good mechanical properties and reasonable oxidation resistance. Unlike many ceramics, these materials have high thermal conductivity which can be advantageous, for example, to reduce thermal shock. Recently, we developed Tersoff style interatomic potentials for both ZrB₂ and HfB₂ appropriate for atomistic simulations. As an application, Green-Kubo molecular dynamics simulations were performed to evaluate the lattice thermal conductivity for single crystals of ZrB₂ and HfB₂. The atomic mass difference in these binary compounds leads to oscillations in the time correlation function of the heat current. Results at room temperature and at elevated temperatures will be reported.